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Short note

Suitable initial conditions

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Abstract

The aim of this note is to draw attention on a computational problem related to the (initial) simulation of very large time-dependant systems. The underlying theoretical problem has been the object of many relevant works in theoretical mathematical, and in the applied literature as well, but it seems that its computational implications are not familiar to many; we hope that this Note will help.

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1. Introduction

Recent discussions with distinguished specialists of numerical fluid mechanics have shown that it would be useful to write a physicist friendly version of the article [14], and this is the aim of this note.

Consider a very simple problem, namely the heat equation in space dimension one:

$$\begin{cases} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f, \quad 0 < x < 1, \ \ t > 0, \\ u(0,t) = u(1,t) = 0, \\ u(x,0) = u_0(x). \end{cases} \tag{1}$$

For u_0 and f given sufficiently regular, "explicit" forms of the solution u of (1) are available using the Green function of the heat equation [2]. Also mathematical results of existence and uniqueness of solutions of (1) are available when f and u_0 are just square integrable, or even less regular [12]. The issues discussed in [14] do not relate to unsmooth data but rather to smooth ones. Assume for instance that $f \equiv 0$, and $u_0(x) = 1$, $\forall x \in (0, 1)$. The existence and uniqueness of solution of (1) is then guaranteed by many theorems, and the solution will be $\mathscr{C}^\infty$ except near $t = 0$. The existence of a discontinuity near $t = 0$ can be seen by just observing that, for f and u_0 as above, $u(0, t) = 0$, for all $t > 0$, whereas $u(0, 0) = u_0(0) = 1$. In fact, assuming that f and u_0 are $\mathscr{C}^\infty$, the

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solution u of (1) will not, in general, be smooth near $t = 0$. It will be so only if (when) u_0 and f satisfy a sequence of conditions called the *compatibility conditions*, the level of regularity near $t = 0$ depending on the number of compatibility conditions that are satisfied. In Section 2 we describe the first and second compatibility conditions (CC) for (1), as well as for the convection and wave equations in space dimension one (the first one for (1) being $u_0(0) = u_0(1) = 0$). As another illustration of the results in [14] we present in Section 3, the substantially more complex case of the Navier–Stokes equations.

The problem of the compatibility conditions has been known and addressed in the mathematical literature for a long time; see e.g. [13] and the references in [14]. The novelty in [14] was to derive *all* the necessary and sufficient conditions for the solutions of certain classes of parabolic equations to be $\mathscr{C}^\infty$ near $t = 0$, and especially the incompressible Navier–Stokes equations.

How this issue relates to computation? From the physical (and somehow "philosophical") point of view, except when considering ab initium problems, any phenomenon considered for $t > 0$ will just be the continuation of a phenomenon which pre-existed, so that we should in principle be able to solve the problem under consideration *backward in time*.[1] Now, for an equation like (1), given f smooth for all $t \in \mathbb{R}$, the u_0 for which (1) can be solved backward are relatively very rare and, for this to be true some (but not all) of the requirements on u_0 are precisely the compatibility conditions. Hence solving (1) with an u_0 which is not physically suitable in this sense, means, despite the beautiful mathematical theorems, that we are trying to solve this problem with a non-physical initial data. There is likely a computational price to pay for that, which is negligible for (1), but is not for more complex equations. For instance those practicing large simulations for the Navier–Stokes equations or geophysical flows, know very well that they have to "prepare" their initial data before launching the actual computations. One may wonder if this "preparation" is not related to making the initial data "suitable" in the sense above. This article does not provide any recipe but, hopefully, by shedding some light on this difficulty, may help the practitioner.

The problem of the choice of initial (and boundary) data has been discussed from many angles, in the applied and computational literature, the compatibility conditions being implicitly or explicitly mentioned. For the Navier–Stokes equations (NSE) the problem of the first and second compatibility conditions has been addressed e.g. by Heywood [9], and Heywood and Rannacher [10]; in [10] the authors emphasize the computational relevance of the compatibility conditions. In his nice book [3], Gallavotti mentions the numerical difficulty caused by an inconsistency in the initial conditions for the NS equations; this difficulty relates to the second compatibility condition (19) below, although the compatibility conditions are not alluded to. See also the book of Kreisz and Lorenz [11] who address related issues (in particular in Chapter 10, Section 10.3.2) in the context of the initialization by "the bounded derivative principle". Several articles of Gresho alone or with co-authors address the initial and boundary conditions issues; see e.g. [4] where the first and second compatibility conditions appear; see also the review articles [5,6]. These issues appear also explicitly in work by Boyd and Flyer [1], Flyer and Fernberg [7], and Flyer and Swarztrauber [8]; see also the references in these articles. These articles emphasize the computational impact of the CC and propose a number of remedies (in particular computing analytically the singularities near $t = 0$, and "removing" them from the solutions).

2. One-dimensional equations

As indicated before we now describe the first and second compatibility conditions for three very simple equations in space dimension one, the first ones being that the initial data satisfies the boundary conditions of the problem, as we already observed in the case of the heat equation.

2.1. Heat equation

As indicated before, u_0 and f are smooth, so that the solution u of (1) is smooth for $t > 0$. We infer from the boundary condition at $x = 0$ that

[1] We realize that this factual remark somehow contradicts the irreversible nature of certain phenomenas, e.g. those described by parabolic equations. Irreversibility reappears however in the fact that one can solve initial boundary value problems for parabolic equations with initial data which *are not* the final value of an anterior phenomenon.

$$-\frac{\partial^2 u}{\partial x^2}(0,t) = f(0,t), \quad t > 0$$

so that, if u is $\mathscr{C}^2$ up to $t = 0$, we must have

$$-\frac{d^2 u_0}{dx^2}(0) = f(0,0). \tag{2}$$

With the similar condition at $x = 1$ and

$$u_0(0) = u_0(1) = 0, \tag{3}$$

we obtain the necessary and sufficient conditions for u to be $\mathscr{C}^2$ up to (near) $t = 0$, see [14].

Remark 1. The case where the boundary conditions in (1) are not homogeneous can be treated in a similar manner. If, instead of (1), we have

$$u(0,t) = g_0(t), \quad u(1,t) = g_1(t), \tag{4a}$$

we can either address this problem directly or reduce it to the case (1) by considering $v(x, t) = u(x, t) - (g_1(t) - g_0(t))(x - 1) - g_1(t)$. We thus obtain the first and second compatibility conditions which read:

$$\begin{cases} u_0(0) = g_0(0) \quad \text{and} \quad u_0(1) = g_1(0), \\ \frac{dg_0(0)}{dt} = \frac{d^2u_0}{dx^2}(0) + f(0,0), \\ \frac{dg_1(0)}{dt} = \frac{d^2u_0}{dx^2}(1) + f(1,0). \end{cases} \tag{4b}$$

Figs. 1–6 show the evolution of the error in space and/or time for the solution u of (1)–(4b) with $f = 0$, $g_0(t) = 1$, $g_1(t) = 0$ and $u_0(x) = x(1 - x)$ so that none of the first and second CC is satisfied at $x = 0$, and the first CC only is satisfied at $x = 1$. On these figures one can observe how significant are the initial errors already induced by the lack of CC for such an elementary problem. A similar example appears in [FF] but many more similar examples can be constructed.

Remark 2. Unlike the wave equations considered in Section 2.2, the heat equation and the Navier–Stokes equation considered in Section 3 relate to *irreversible* phenomena, so that, physically, it is not thinkable to consider the resolution of these equations backward in time. Nevertheless as explained in Section 1 and as it appears in this equation, the past does exist and somehow reflects itself in the compatibility conditions.

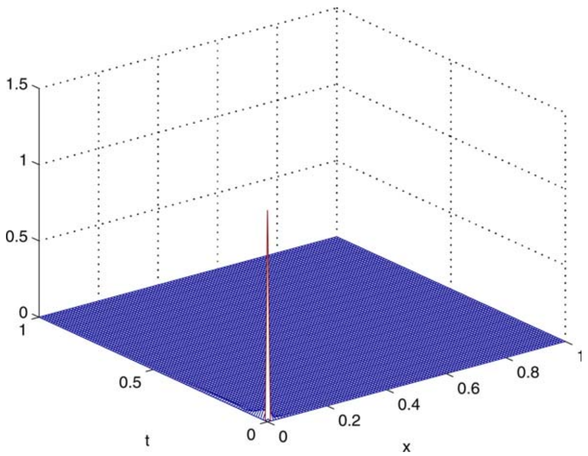

Fig. 1. Pointwise error, $0 < x < 1$, $0 < t < 1$, with timestep = 0.001, spacestep = 0.001.

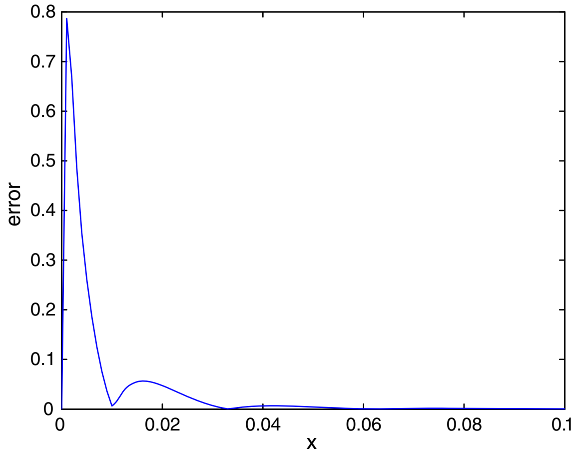

Fig. 2. Pointwise error, at $t = 0.01$, $0 < x < 0.1$.

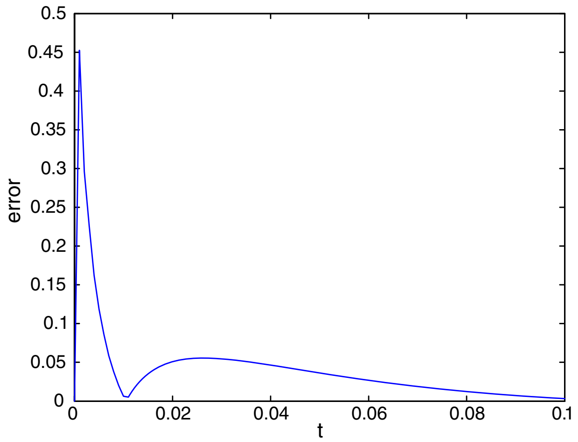

Fig. 3. Pointwise error, at $x = 0.01$, $0 < t < 0.1$.

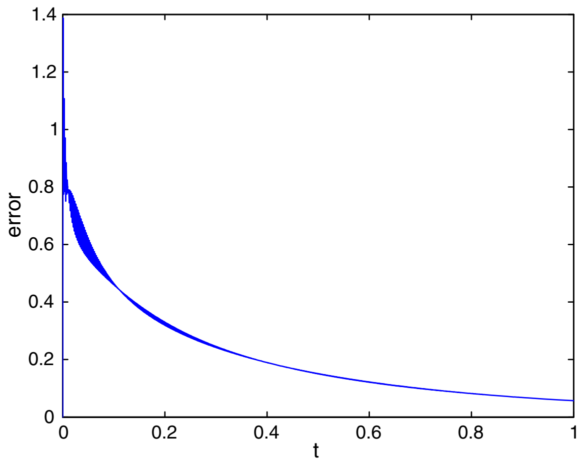

Fig. 4. Time evolution of the maximum error.

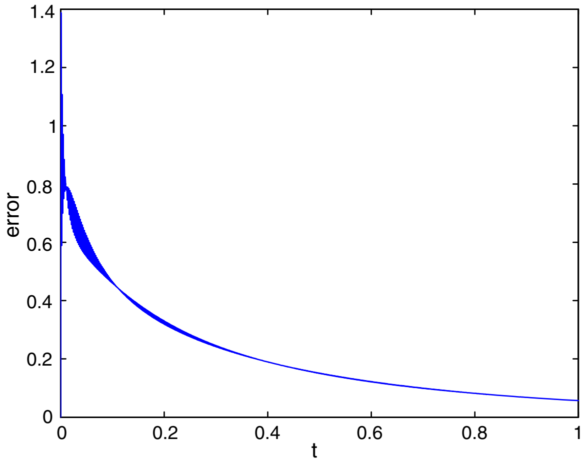

Fig. 5. Time evolution of the error along the left boundary.

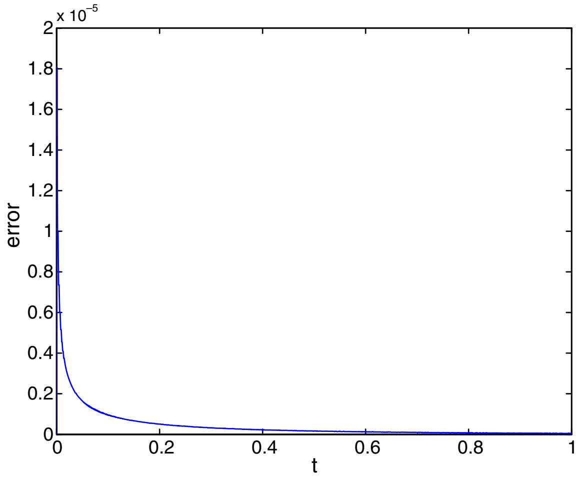

Fig. 6. Time evolution of the error along the right boundary.

2.2. Convection and wave equations

Consider the problem

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = f, \quad 0 < x < 1, \ \ t > 0, \\ u(0, t) = 0, \\ u(x, 0) = u_0(x). \end{cases} \tag{5}$$

This problem is well-posed for f and u_0 smooth and we have

$$\frac{\partial u}{\partial x}(0, t) = f(0, t), \quad t > 0,$$

so that, if u is smooth near $t = 0$, then

$$\frac{\mathrm{d}u_0}{\mathrm{d}x}(0) = f(0, 0). \tag{6}$$

Together with

$$u_0(0) = 0, \tag{7}$$

we obtain the necessary and sufficient conditions for u to be $\mathscr{C}^1$ near $t = 0$; see [13].

Finally, consider the 1D wave equation

$$\begin{cases} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = f, \quad 0 < x < 1, \ t > 1, \\ u(0,t) = u(1,t) = 0, \\ u(x,0) = u_0(x), \quad \frac{\partial u}{\partial t}(x,0) = u_1(x), \ 0 < x < 1. \end{cases} \tag{8}$$

As before we see that if u is $\mathscr{C}^2$ near $t = 0$, then necessarily

$$\begin{cases} u_0(0) = u_0(1) = u_1(0) = u_1(1) = 0, \\ -\frac{d^2 u_0}{dx^2}(0) = f(0,0), \quad -\frac{d^2 u_0}{dx^2}(1) = f(1,0), \\ -\frac{d^2 u_1}{dx^2}(0) = \frac{\partial f}{\partial t}(0,0), \quad -\frac{d^2 u_1}{dx^2}(1) = \frac{\partial f}{\partial t}(1,0). \end{cases} \tag{9}$$

Conversely, it is shown in [14] that if u_0, u_1, f are smooth and satisfy (9) then u is $\mathscr{C}^2$ near $t = 0$.

3. Generalization: Navier–Stokes equations

In this section, we present the general form of the compatibility conditions and then consider the special case of the Navier–Stokes equations.

3.1. Generalization

Let Ω be a domain of $\mathbb{R}^d$ with boundary $\partial\Omega$ and let u be a scalar or vector solution of a partial differential equation

$$\frac{\partial u}{\partial t} + P(D)u = f \quad \text{in } \Omega \times (0,T), \tag{10}$$

where $P(D)$ is a linear spatial differential operator. If u is smooth then, by successive time differentiation of (10), one can compute all time derivatives of u in terms of spatial derivatives of u and f up to the boundary:

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial f}{\partial t} - P(D)\frac{\partial u}{\partial t} = \frac{\partial f}{\partial t} - P(D)[f - P(D)u], \tag{11}$$

etc. If u is smooth up to $t = 0$ and, say, u vanishes on some part Γ_0 of $\partial\Omega$, then

$$\begin{cases} u_0 = 0 \quad \text{on } \Gamma_0, \\ [f - P(D)u_0] = 0 \quad \text{on } \Gamma_0, \\ \frac{\partial f}{\partial t} - P(D)f|_{t=0} + P(D)^2 u_0 = 0 \quad \text{on } \Gamma_0, \ \text{etc.} \end{cases} \tag{12}$$

The conditions $(12)_1$–$(12)_3$ are the first, second and third compatibility conditions on u_0 and f, and are necessary, for u to be $\mathscr{C}^0, \mathscr{C}^1, \mathscr{C}^2$ near $t = 0$. The kth compatibility condition necessary for u to be $\mathscr{C}^k$ near $k = 0$ reads

$$\frac{\partial^k u}{\partial t^k}(x,0) = 0, \quad x \in \Gamma_0, \ t = 0, \tag{13}$$

where the left-hand side of (13) has been expressed as in (11) in terms of u_0 and its spatial derivatives, and f and its time and spatial derivatives.

Showing that these conditions are necessary has been easy; showing that they are necessary has been done in [13] for hyperbolic equations and in a number of references for parabolic or wave equations; see also [14].

Although the brief presentation in this section is for a linear partial differential equations, the approach applies also to nonlinear problems with of course some additional technical difficulties and we now consider the case of the Navier–Stokes equations.

3.2. Navier–Stokes equations

The remarkable feature of the compatibility conditions for the Navier–Stokes equations is that, due to the incompressibility condition and the presence of the pressure, these CC are *global in nature*.

Consider the Navier–Stokes equations (NSE) in the smooth bounded domain Ω of $\mathbb{R}^d, d = 2$ or 3, with no-slip boundary condition on $\partial\Omega$:

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} - \nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mathbf{f}, & x \in \Omega, \ t > 0, \\ \operatorname{div} \mathbf{u} = 0, & x \in \Omega, \ t > 0, \\ \mathbf{u} = 0 \quad \text{on } \partial\Omega, \\ \mathbf{u}(x,0) = \mathbf{u}_0(x), & x \in \Omega. \end{cases} \tag{14}$$

The mathematical theory of the NSEs makes use of the space

$$H = \{\mathbf{v} \in L^2(\Omega)^d, \quad \operatorname{div} \mathbf{v} = 0, \qquad \mathbf{v}\cdot\mathbf{n} = 0 \quad \text{on } \partial\Omega\},$$

with $\mathbf{n}$ the unit outward normal on $\partial\Omega$. By projecting the first equation (14) onto the space H we obtain (see e.g. [15]), the weak (Leray) form of the system:

$$\begin{cases} \frac{d\mathbf{u}}{dt} + \nu A\mathbf{u} + B(\mathbf{u},\mathbf{u}) = \mathbf{f}, \\ \mathbf{u}(0) = \mathbf{u}_0, \end{cases} \tag{15}$$

where $A\mathbf{u} = -P\Delta\mathbf{u}$, $B(\mathbf{u},\mathbf{u}) = P((\mathbf{u}\cdot\nabla)\mathbf{u})$, and P is the Helmholtz–Leray projection from $\mathbf{L}^2(\Omega)^d$ onto H and $\mathbf{f} = P\mathbf{f}$ for simplicity (that is $\operatorname{div}\mathbf{f} = 0$, and $\mathbf{f}\cdot\mathbf{n} = 0$ on $\partial\Omega$). One can solve the initial value problem (14) and (15), at least locally in time, for $\mathbf{u}_0 \in H$ (see [15]). For more regularity at $t = 0$, we will require that

$$\mathbf{u}_0 \in V = \{\mathbf{v} \in H_0^1(\Omega)^d, \quad \operatorname{div} \mathbf{v} = 0\}. \tag{16}$$

Here, $H_0^1(\Omega)$ is the Sobolev space of functions in $L^2(\Omega)$ with first derivatives in $L^2(\Omega)$ and which vanish on $\partial\Omega$; (16) is the first CC for the Navier–Stokes equations. The second CC is that

$$\left.\frac{d\mathbf{u}}{dt}\right|_{t=0} = P\mathbf{f}(0) - B(\mathbf{u}_0,\mathbf{u}_0) - \nu A\mathbf{u}_0 \in V. \tag{17}$$

Since the right-hand side of (17) is divergence free, the only requirement in (17) (see [14]), is that the right-hand-side of (17) vanishes on the boundary $\partial\Omega$. Define the function p_0 (*the initial pressure*) by solving the Neumann problem

$$\Delta p_0 = \sum_{i,j=1}^{d} \frac{\partial u_{0i}}{\partial x_j}\frac{\partial u_{0j}}{\partial x_i} \quad \text{in } \Omega,$$

$$\frac{\partial p_0}{\partial \mathbf{n}} = \mathbf{n}\cdot(\nu\Delta\mathbf{u}_0) \quad \text{on } \partial\Omega.$$

Then the right-hand side of (17) is equal to

$$\mathbf{f}(\cdot,0) + \nu\Delta\mathbf{u}_0 - (\mathbf{u}_0\cdot\nabla)\mathbf{u}_0 - \nabla p_0. \tag{18}$$

Since the normal component of (18) on $\partial\Omega$ vanishes by definition of p_0, the condition is then that

$$\begin{aligned} &\textit{The tangential component of } \nabla p_0 \quad \text{on } \partial\Omega \textit{ is equal} \\ &\textit{to the tangential component of } \nu\Delta\mathbf{u}_0 + \mathbf{f}(\cdot,0). \end{aligned} \tag{19}$$

This is the second compatibility condition for the Navier–Stokes equations [14], appearing as well in the references quoted above [9,10,3(Section 2.1.3),4].

4. Remarks and conclusions

(i) The higher order compatibility conditions for the Navier–Stokes equations appear in [14] (in an abstract (mathematical) form).

(ii) The difficulty described here has nothing to do with the question of occurrence of singularities in finite time for the 3D Navier–Stokes equation. Our analysis relates to smooth data and solutions that are smooth for $t > 0$.

(iii) Returning to the computational problem, the unavoidable issue is, for a general $\mathbf{u}_0$ not satisfying (19), to solve an exact or approximate form of the Navier–Stokes equation with this initial data $\mathbf{u}_0$ until $\mathbf{u}(\cdot, t)$ satisfies (19) for some $t_0 > 0$, after what $\mathbf{u}(\cdot, t_0)$ will be the actual initial data. Finding non-costly procedures of this type remains an open question. It may relate to the "preparation" of the initial data mentioned in Section 1.

(iv) We conclude this note with an erratum for [14]: (1.11) read: "and H is a closed subspace of E_0" (instead of $H = E_0$); (1.14) reads: $\mathscr{A}$ is an isomorphism from $E_{m+2} \cap V_2$ onto $E_m \cap H$, $\forall m \geqslant 0$; (1.16), read: $\forall u \in E_{m+2} \cap V_2, m \geqslant 0$. In the definition of W_m at the bottom of page 76 read "$v \in \mathscr{C}([0, T]; E_m \cap H)$" instead of "$v \in \mathscr{C}([0, T]; E_m)$"; (1.20) reads "$u \in \mathscr{C}([0, T]; E_m \cap H)$". The first sign in (1.23) is $+$ instead of $-$. The second proof of Theorem 2.1 in Section 2.3 is not valid at this level of generality and is withdrawn.

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